CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: The 9th International Symposium of the Functionally Graded Materials
Project # 20.06002.01.342
AI # 20.06002.01.342.701

DATE/PLACE: October 15–18, 2006
Ko Olina, Hawaii

AUTHOR: Fernando Ferrante

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PERSONS PRESENT:

Attendance at the 9th International Symposium of the Functionally Graded Materials (FGM) was estimated at 200 participants during the opening lecture on October 16, 2006. These mainly included academic researchers from the fields of micromechanics, computational mechanics, multiscale, multiphysics, and composite manufacturing.

BACKGROUND AND PURPOSE OF TRIP:

The event is part of biennial conferences supervised by the International Advisory Committee on FGM (IACFGM) in conjunction with the International Scientific Committee (ISC). This year's conference was sponsored and organized by the University of Illinois at Urbana-Champaign (UIUC) and the Federal University of Rio de Janeiro (UFRJ).

The technical program consisted of a short course, 5 plenary lectures, 23 mini-symposia spread over 53 sessions, and a poster session for graduate students. The conference proceedings will be published in book form in a few months, and authors of outstanding papers will be invited to publish extended papers in either the International Journal of Plasticity or the Multiscale Computational Engineering Journal. A book of abstracts was provided at the conference.

Specific purposes for attending the meeting were to

- Fulfill a special invitation by one of the co-chairs of the conference (M.-J. Pindera from the University of Virginia) to deliver a 40-minute keynote lecture titled "An Overview of Micromechanics-Based Techniques for the Analysis of Microstructural Randomness in FGM" in the mini-symposium "Micromechanics of Multiphase and Graded Materials"

- Attend technical sessions on various topics outlined in the next section

SUMMARY OF PERTINENT POINTS:

The theme of this year's conference was expanded from the traditional functionally graded materials theme to include multiscale and multiphysics topics. The mini-symposia were divided into 23 topics ranging from modeling and simulation to processing and characterization of functionally graded materials. A significant number of presentations were made in the area of

graded cementitious composites, which have flourished as an avenue of research for functionally graded materials in recent years.

The five plenary lectures highlighted the breadth of the conference. Jacob Fish from Rensselaer Polytechnic Institute (who also delivered the short course) presented an update on some of his distinguished work in multiscale and multiphysics problems with the presentation of "Design Impact, Fragmentation and Fatigue of Composite Materials and Structures.". Yoshinari Miyamoto from Osaka University in Japan gave a plenary lecture on the state-of-the-art processing and computer-aided design of functionally graded materials titled "Computer-aided Design and Processing of Functionally Structured and Graded Materials." Emilio C.N. Silva from the University of São Paulo in Brazil discussed topology issues while presenting "Design of functionally graded piezoelectric multiactuated microtools using topology optimization." Biological functionally graded materials were the subject of Winston Soboyejo from Princeton University, titled "Bioinspired Design of Functionally Graded Material Systems." Finally, Monika Willert-Porada from the University of Bayreuth in Germany discussed fabrication issues in an overview entitled "Design and Fabrication Principles in the Natural and Technical World of Graded Functionality."

Jacob Fish presented a full-day short-course on multiscale and multiphysics. This included motivation and background of multiscale problems in science and engineering with an emphasis on the issues involving heterogeneous materials and functionally graded materials. An overview on the history and current approaches on a particular technique titled "Spatial Scales Decomposition" were also presented. Several topics were discussed in detail, including modeling errors resulting from bridging different scales, multiscale sensitivities, discrete-to-continuum bridging methods, and multiple temporal scales. Finally, the Concurrent Multiscale Approach, based on extensive work by Fish and others, was introduced and discussed.

The full list of authors and the conference program are available at the website maintained by UIUC: http://cee.uiuc.edu/events/FGM2006. The specific presentations discussed below were attended by the author of this trip report and are mentioned here in more detail.

Sinisa Mesarovic from Washington State University discussed continuum and network modeling approaches to the multiscale bridging problem in his presentation titled "Transition Between the Models in Multiscale Simulations: Continuum and Network Models." The issue of information passing between coarse-scale and fine-scale was tackled by the introduction of a mathematical concept called Minimal Boundary Conditions, which is developed to address the lack of localization of stress/strain fields and other issues arising in currently available methods. Application of the concept to kinematic and static boundary conditions was implemented for granular materials in conjunction with discrete finite element modeling.

Marc Ingber from the University of New Mexico considered potential limitations in the use of effective properties for composite materials, including functionally graded materials. The derivation of a third effective elastic property based on the commonly used two independent effective elastic properties (Young's modulus and Poisson's ratio) for homogeneous elastic isotropic materials was questioned in terms of its extension to heterogeneous materials. Numerical examples of the limitations were provided by comparison of effective properties with a simulation of boundary conditions on mesoscopic samples of composite materials.

Linfeng Chen from the University of Virginia discussed microstructural effects in finite multilayers with single and multiple aligned cracks. His work expanded on a recently developed elastic solution that exactly accounts for finite multilayered domains in generalized plane strain deformation weakened by the inclusion of aligned cracks. Crack opening shape conversion, degradation of elastic properties, and the presence of cracks in either the soft or hard layer of the composite were investigated using numerical samples of laminated materials.

Philippe Geubelle (UIUC) introduced computational modeling work to simulate the dewetting phenomenon in particulate composites, which is a damage process resulting in the debonding between particle and matrix in a specific category of composite materials. This effect was identified as a major contributor to crack propagation in highly filled particulate composites such as solid propellant and other energetic materials. A multiscale finite element framework developed by the author that includes nonlinear material behavior of the matrix phase and cohesive modeling of the damage was discussed. Its application was demonstrated for the case of a highly filled particulate composite with spherical inclusions of random sizes.

Anthony Drago from Sikorsky Aircraft Company in Connecticut provided an overview of his work on the homogenization approach to computational modeling of periodic heterogeneous materials. The distinction between two commonly used homogenization concepts, the repeating unit cell (RUC) and the representative volume element (RVE), were discussed in terms of their applications to predict the response of statistically homogeneous composites and periodic composites. As an example, exact localized elasticity solutions were implemented for the periodic class of materials, with closed-form solutions derived for the homogenized moduli of unidirectionally-reinforced heterogeneous composites.

The author of this report presented an invited keynote lecture titled "An Overview of Micromechanics-Based Techniques for the Analysis of Microstructural Randomness in Functionally Graded Materials" (see the attached abstract). An overview of the current state of knowledge in micromechanical studies that incorporate randomness due to microstructure effects was provided with the inclusion of a probabilistic framework developed by the author for his doctoral thesis. Exposition of both the overview and the work performed at Johns Hopkins University previous to joining the Center for Nuclear Waste Regulatory Analyses was well received.

CONCLUSIONS:

The participation in the 9th International Symposium of the Functionally Graded Materials was a highly beneficial way to interact with researchers in the multiscale, multiphysics, and functionally graded materials community. The invited keynote lecture delivered by the author was an opportunity to expose his expertise to a wider and distinguished audience.

PROBLEMS ENCOUNTERED:

None.

PENDING ACTIONS:

None.

RECOMMENDATIONS:

Continued involvement in current and future activities involving multiscale, multiphysics, and/or FGM related to nuclear applications is highly recommended.

SIGNATURE:

Fernando Ferrante, Research Engineer
Mining, Geotechnical, and
Facility Engineering

11/18/2006
Date

CONCURRENCE:

Asadul H. Chowdhury, Manager
Mining, Geotechnical, and
Facility Engineering

11/13/2006
Date

Sitakanta Mohanty, Assistant Director
Engineering and Systems Assessment

11/13/2006
Date

ATTACHMENT

ABSTRACT

AN OVERVIEW OF MICROMECHANICS-BASED TECHNIQUES FOR THE ANALYSIS OF MICROSTRUCTURAL RANDOMNESS IN FUNCTIONALLY GRADED MATERIALS

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Randomness in microstructure, which is inherent to functionally graded composites, can exhibit considerable challenges in the development of practical and theoretical tools to efficiently characterize their material properties. While gradients are introduced to optimize combinations of dissimilar materials through a gradual change in physical characteristics, an increased level of complexity is required during the manufacturing process in order to achieve smooth transitions. This added difficulty can result in material property variations that deviate considerably from their expected gradients. Hence, attention has been aimed at characterizing the effect of variations on the mechanical response of functionally graded materials.

The objective of this presentation is to provide an overview of these efforts, focusing on the micromechanical techniques developed for material characterization including microstructural randomness of FGM. For example, one approach consists in deriving the overall constitutive equations of the material through micromechanics-based assumptions in order to account for statistical non-uniform heterogeneity of the material field response i.e., [1], [2], and [3]. Another related method is the use of algorithms that either generate or reconstruct samples of FGM, by including microstructural detail such as inclusion shape and size i.e., [4] and [5]. In either case, any assumptions based on geometry are usually very difficult to generalize.

An alternative is to consider digitized microstructural images as a basis for the analysis where structure detail is not required *a priori* and approximate results offer solutions to complex problems that are otherwise intractable. This general approach, developed for uniform randomly distributed composites i.e., [6], [7], and [8] was extended to functionally graded materials by the authors, through a combination of probabilistic methods and microstructural characterization of random media using a robust homogenization method i.e., [9] and [10] with a moving-window technique [8] to evaluate randomness effects. The flexibility of the approach allows for the analysis of samples generated both through geometric-based assumptions and samples synthesized from a novel probabilistic approach [11] that reproduces the interconnectedness (percolation) of functionally graded materials that do not exhibit clearly defined inclusions. The

efficiency of the method with respect to the analysis of randomness effects in functionally graded materials will be discussed.

ACKNOWLEDGMENT

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